Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

10 April 2012

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Updates to Pleiades Improve System Reliability

- The HECC Supercomputing Systems team took advantage of a scheduled dedicated time (in preparation for the addition of 24 new racks of Sandy Bridge processors) to make several improvements to the Pleiades supercomputer:
  - Updated the InfiniBand software; the new release provides support for Fourteen Data Rate (FDR) InfiniBand, with speeds of 54 gigabits per second
  - Configured Quality of Service on InfiniBand to provide bandwidth guarantees to key services (Lustre, Message Passing Interface, and IP over InfiniBand)—this ensures that all services get a fair share of the network bandwidth
  - De-installed 28 Harpertown compute racks to provide physical space for the new Sandy Bridge racks
  - Successfully tested the suspension and resumption of PBS batch jobs; this feature allows some maintenance activities to occur without impacting running jobs
  - Updated the InfiniBand Subnet Manager, the Portable Batch System, and the NAS File System servers.

Mission Impact: The improved system reliability and performance gained from regular upgrades provides HECC users with a more usable computational capability.

Figure: Dedicated time on the Pleiades supercomputer (above) enabled HECC staff to improve ongoing system operations.

POC: *Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.s.chan@nasa.gov, (650) 604-4613, NASA Advanced Supercomputing Division, Computer Sciences Corp.*

Cable-Lift Structure on Computer Floor Facilitates Upgrade, Reduces Downtime

- In preparation for installation of the Sandy Bridge nodes on Pleiades, HECC engineers devised an ingenious cable-lift system to facilitate removal of older racks located in the middle of the computer floor.
- The engineers designed and installed a structure to accommodate this lift without interrupting production computing.
- The structure was attached to the tops of adjacent 2700-lb. racks, which provided ample anchorage.
- Once the old racks were shut down, the cable lift was accomplished without any interruption.
- The cables will remain in this lifted configuration until the new racks are installed, and will then be lowered and the structure removed.

Mission Impact: Devising creative methods for efficiently and effectively handling facilities tasks related to expansion of HECC computing resources allows users to continue running jobs for all Mission Directorates without interruption.

Figures: Twelve groups of cables are shown suspended from the cable-lift structure, as part of the process for expanding the Pleiades supercomputer.

POC: *John Parks, john.w.parks@nasa.gov, (650) 604-4225, NASA Advanced Supercomputing Division*

Large-Memory Nodes Deployed on Pleiades Enable More Efficient Performance

- The HECC Supercomputing Systems team deployed large-memory nodes on Pleiades to support users who are running jobs with larger memory requirements.
- Four Westmere nodes were quadrupled to 96 gigabytes (GB) of memory, and another 16 nodes were doubled to 48 GB of memory; these nodes are spread across the whole system to utilize them more effectively.
- Typically, a large-memory node for I/O is used by the master process, with the rest of the processes running on "regular" (24 GB) nodes.
- The success of this usage model is demonstrated by the recent 6–7x speedup of the Enzo application attained by Science Mission Directorate user Renyue Cen.
- Availability of these large-memory nodes also enabled Aeronautics Research Mission Directorate user Mehdi Khorrami to evaluate various aircraft noise reduction concepts by using higher fidelity cases that were previously impossible with the regular nodes.

Mission Impact: New large-memory nodes enable HECC users to more efficiently perform large I/O or memory-intensive calculations—in some cases, performing computations that were previously impossible to run on Pleiades.

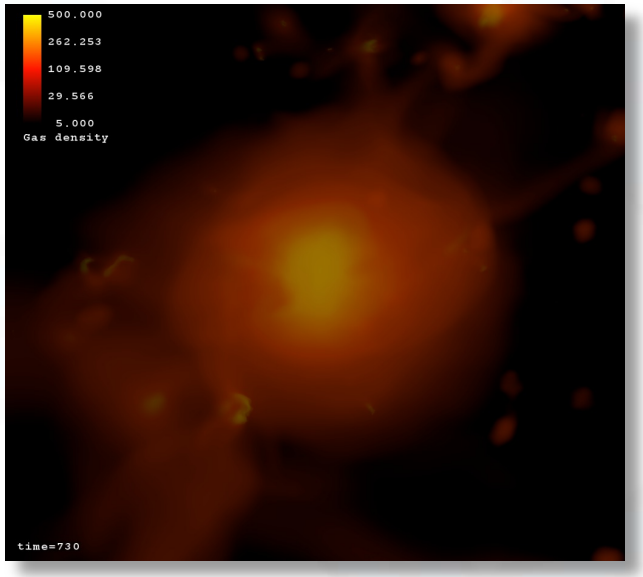


Figure: Close-up of a galaxy cluster from one of 1,561 time steps, each with 8 to 13 gigabytes of data, generated from an Enzo simulation on Pleiades. (David Ellsworth, NASA/Ames)

POC: *Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.s.chan@nasa.gov, (650) 604-4613, NASA Advanced Supercomputing Division, Computer Sciences Corp.*

Pleiades Unofficially Ranks 2nd Among World's Fastest Supercomputers on Graph500

- After the Pleiades dedicated time activities, (see slide 3), Intel systems engineers ran the Graph500 benchmark on 1,024 Westmere nodes and achieved 192 billion traversed edges per second (TEPS), which would unofficially place the system as the 2nd fastest on the current Graph500 list.
- The Graph500 is a graph benchmark designed to measure the performance of data-intensive supercomputer applications; established in 2010, the list is updated semi-annually in November and June and complements the LINPACK benchmark (used for the TOP500) to provide a more complete view of a system's performance.
- Running the Graph500 benchmark provided valuable information that will be used to help guide future software updates to provide better scaling performance.

Mission Impact: Through the HECC Project, NASA science and engineering users have access to a well balanced computing system to run a wide variety of NASA's data-intensive applications.

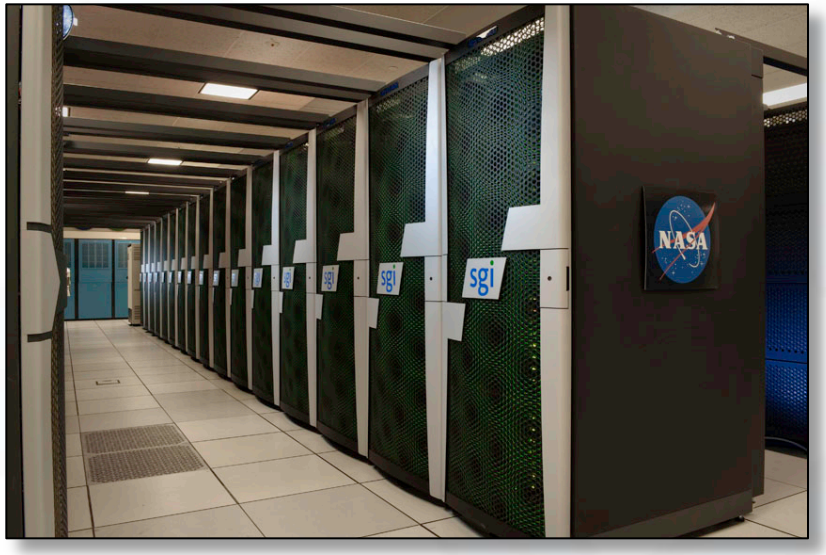


Figure: *HECC systems engineers achieved 192 billion traversed edges per second on the Graph500 benchmark, running 1,024 Westmere nodes (16 racks) on Pleiades.*

POC: *Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.s.chan@nasa.gov, (650) 604-4613, NASA Advanced Supercomputing Division, Computer Sciences Corp.*

Optimization Work Yields 80x Speedup on Code Using Goddard Cumulus Ensemble

- HECC computational specialists completed the implementation of a project to increase both the scalability and performance of the Goddard Multi-scale Modeling Framework.
- Benchmarks show an 80-fold speedup in code execution, using 4,350 cores on Pleiades.
- NASA Goddard researchers turned to HECC when progress was slowed due to the enormous computational requirements and limited scalability of their 2D cloud model (no more than 30 cores).
- The Goddard researchers are already considering the potential for using higher resolution (3D) models—something that would have been unthinkable at previous performance levels.

Mission Impact: By improving computational performance of the Goddard Multi-Scale Modeling Framework, HECC enables the use of better and more accurate climate simulation models for NASA Science Mission Directorate programs and projects.

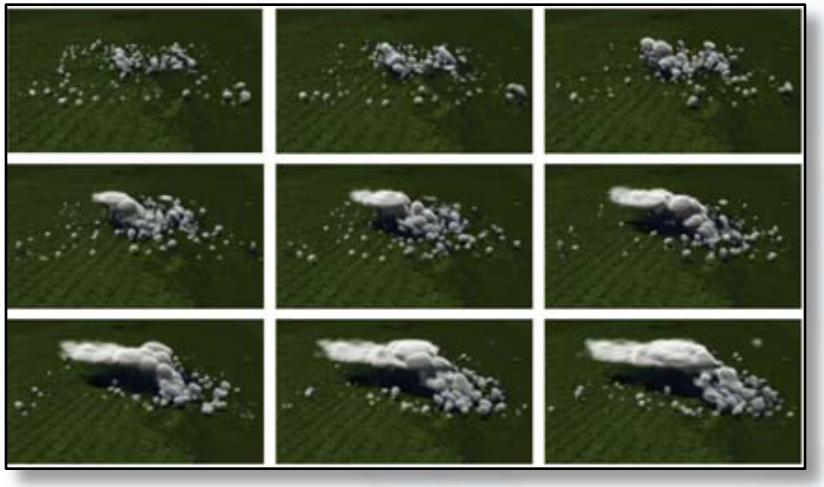


***Figure**: Cloud formation modeling using the Goddard Cumulus Ensemble. This series of images shows a computer prediction of cloud formation.*

***POCs:** Bron C. Nelson, bron.c.nelson@nasa.gov, (650) 604-4329, NASA Advanced Supercomputing Division, Computer Sciences Corp.; Bo-wen Shen, bo-wen.shen-1@nasa.gov, (301) 614-6251, NASA Goddard Space Flight Center/University of Maryland.*

New e-Books Tailored to Support Collecting Requests for Supercomputer Time

- The e-Books system used by NASA Mission Directorates to collect and manage requests for supercomputer time has been updated and modernized.
- The new version of e-Books was released for production February 29, 2012—in time to begin collecting requests for the allocation period that begins May 1.
- The new e-Books eliminates many of the difficulties users encountered with the previous version, which was developed for a different purpose. New features and benefits include:
  - Users can now log in to just one place to submit a request to any Mission Directorate.
  - Information summarizing the status of each request is clearly indicated with color and text messages.
  - Navigation tabs were added and information can be periodically saved and then reviewed with the "Review/Submit" tab.
- Future versions will provide statistics about the submissions.

Mission Impact: With a modernized web-based system, Mission Directorates are able to collect more information about computing requests, do so in a more consistent and usable manner, and maintain a history of requests from year to year.

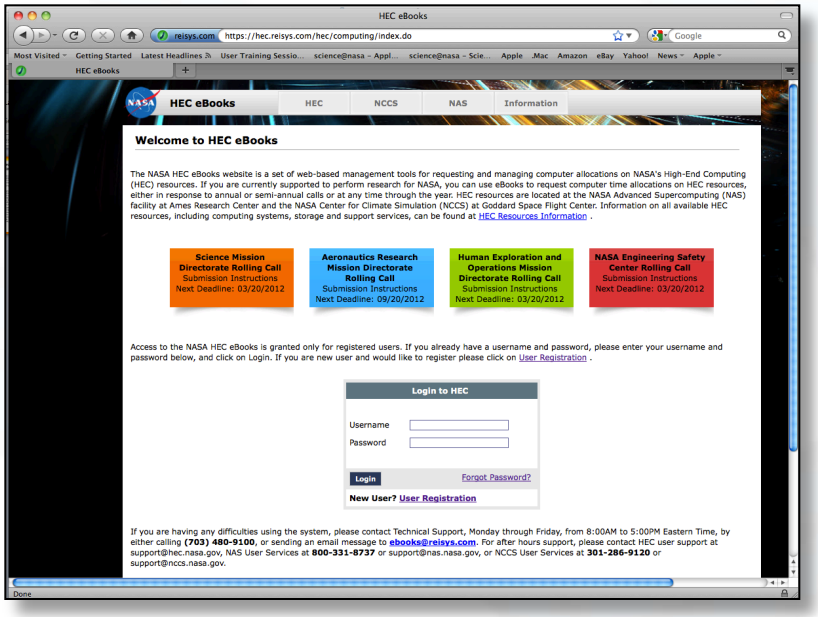


Figure: Screen shot of main page for logging into e-Books to submit computing requests for any of NASA's Mission Directorates and the NASA Engineering and Safety Center. See: https://hec.reisys.com/hec/computing/index.do

POC: *Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division*

Network Team Releases Technical Whitepaper on Flow Analysis Tool

- The HECC Network team has published a whitepaper explaining its flow-collection techniques and methods for integrating flow data to enable automated performance analysis.
- Using standard open source software, the team created a flexible back-end infrastructure and populated it with data polled from multiple sources that capture key information:
  - Who the user is transferring data to;
  - Any end-to-end network congestion;
  - Whether the remote system is optimally tuned;
  - Any bottlenecks in the network, application, or system.
- The paper also details options for a front-end web interface to easily track, manage, and log flow information and to automatically identify poorly performing transfers, based on a custom-defined algorithm.
- Additional options include visualization of flow data, including the team's Network Diagnostic Tool and Network Path and Application Diagnosis measurement reports, and meta (e.g. per site) analysis capabilities.

Mission Impact: The Flow Analysis Tool allows HECC network staff to proactively identify performance bottlenecks by analyzing key protocol parameters captured directly from user's flows; release of this whitepaper provides information to the IT community regarding how this tool was developed and implemented.

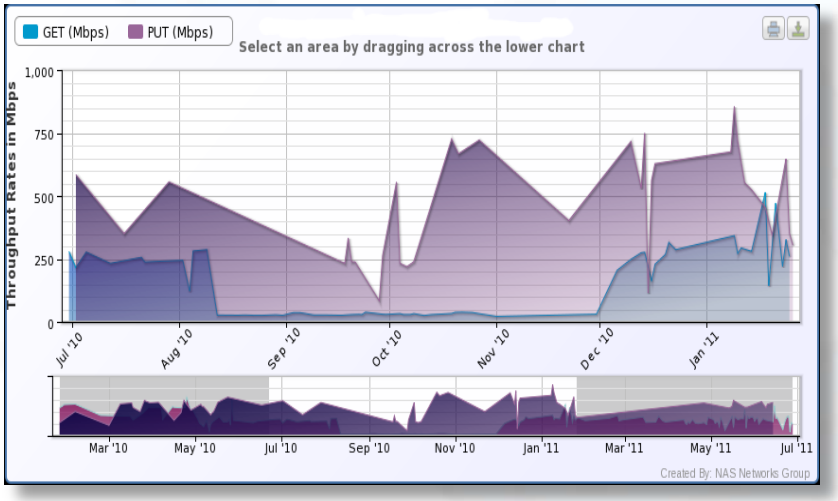


Figure: The above diagram illustrates an asymmetric performance problem during a period when a remote network change was made, which was then identified by NAS engineers and resolved.

POC: *Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.*

Simulations of the Solar Atmosphere: 'Sun in a Box'*

- To understand how the Sun's atmosphere is shaped and heated, and how it impacts Earth, researchers supporting NASA's Science Mission Directorate are simulating a small portion of the Sun in a computational 'box' six times the size of Earth.
- The research team's advanced, multi-dimensional, radiative magnetohydrodynamic simulations of the solar atmosphere have provided new insight into:
  - How the outer solar atmosphere is heated to temperatures much higher than the Sun's surface through the dissipation of magnetic field energy;
  - How the complex interactions of magnetic fields, hydrodynamics, and radiation fields shape the Sun's atmosphere;
  - How small-scale magnetic fields impact the low solar atmosphere, and how magnetic waves help power the solar wind.
- Numerical modeling of the Sun's complex radiative transfer and physical processes, combined with the enormous contrasts of densities, temperatures, and magnetic fields within the solar atmosphere, demands the massively parallel capabilities of the Pleiades supercomputer.

Mission Impact: Enabled by the Pleiades supercomputer's parallel processing capabilities, solar simulations are crucial to interpreting images of the sun's atmosphere obtained from current NASA missions such as the Solar Dynamics Observatory and the Interface Region Imaging Spectrograph (IRIS) explorer, launching in December 2012.

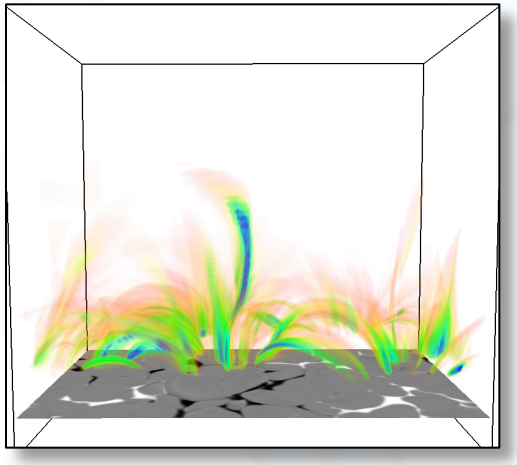


***Figure**: Snapshot from a recent simulation shows how the Sun's outer atmosphere (corona) is heated to millions of degrees through the dissipation of electrical currents (shown in color) created by stressing the magnetic field (shown in gray scale) in the Sun's interior or convection zone. The heating occurs at lower heights than previously thought. Viggo Hansteen, University of Oslo*

***POC:** Bart De Pontieu, bdp@lmsal.com, (650) 424-3094, Lockheed-Martin Solar and Astrophysics Lab; Mats Carlsson, mats.carlsson@astro.uio.no, University of Oslo*

** HECC provided supercomputing resources and services in support of this work.*

HECC Resources Enable Timely Insights for Supersonic Nozzle Design Process*

- Enabled by HECC supercomputing resources, researchers at NASA Glenn are investigating innovative nozzle concepts for commercial supersonic transport, with a goal to reducing noise at takeoff while maintaining high thrust.
- Reynolds-Averaged Navier-Stokes (RANS) computational fluid dynamics (CFD) simulations support aerodynamic screening of the concepts and provide necessary inputs for noise prediction codes. Outcomes include:
  - Updates to the Wind-US CFD code's structured and unstructured solvers resulted in closer agreement with test data, leading to better inputs for noise prediction;
  - The validated unstructured solver within Wind-US provides another tool to increase engineering and computation efficiencies for complex nozzles;
  - Analyses performed with the RANS CFD method helped screen and map out the design space for integration of various noise-suppression technologies into complex nozzles.
- Access to Pleiades enables researchers to obtain timely insights during the conceptual design process; large amounts of data storage and high-speed networks have been essential for the complex, grid-intensive cases.

Mission Impact: Adding to the arsenal of tools for use with complex nozzle geometries increases engineering and computation efficiencies. Screening complex nozzle geometries with CFD is a critical first step prior to fabricating costly test hardware.

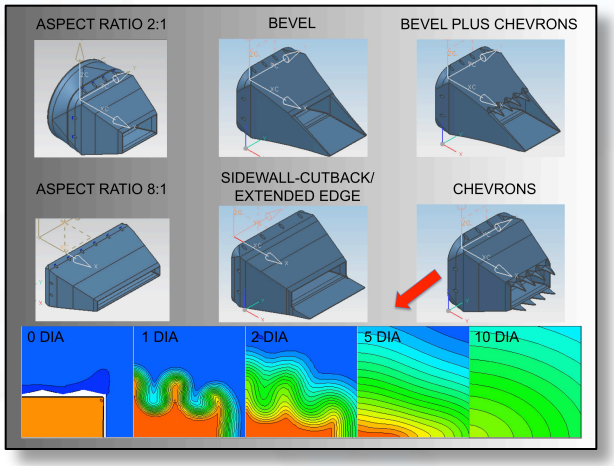


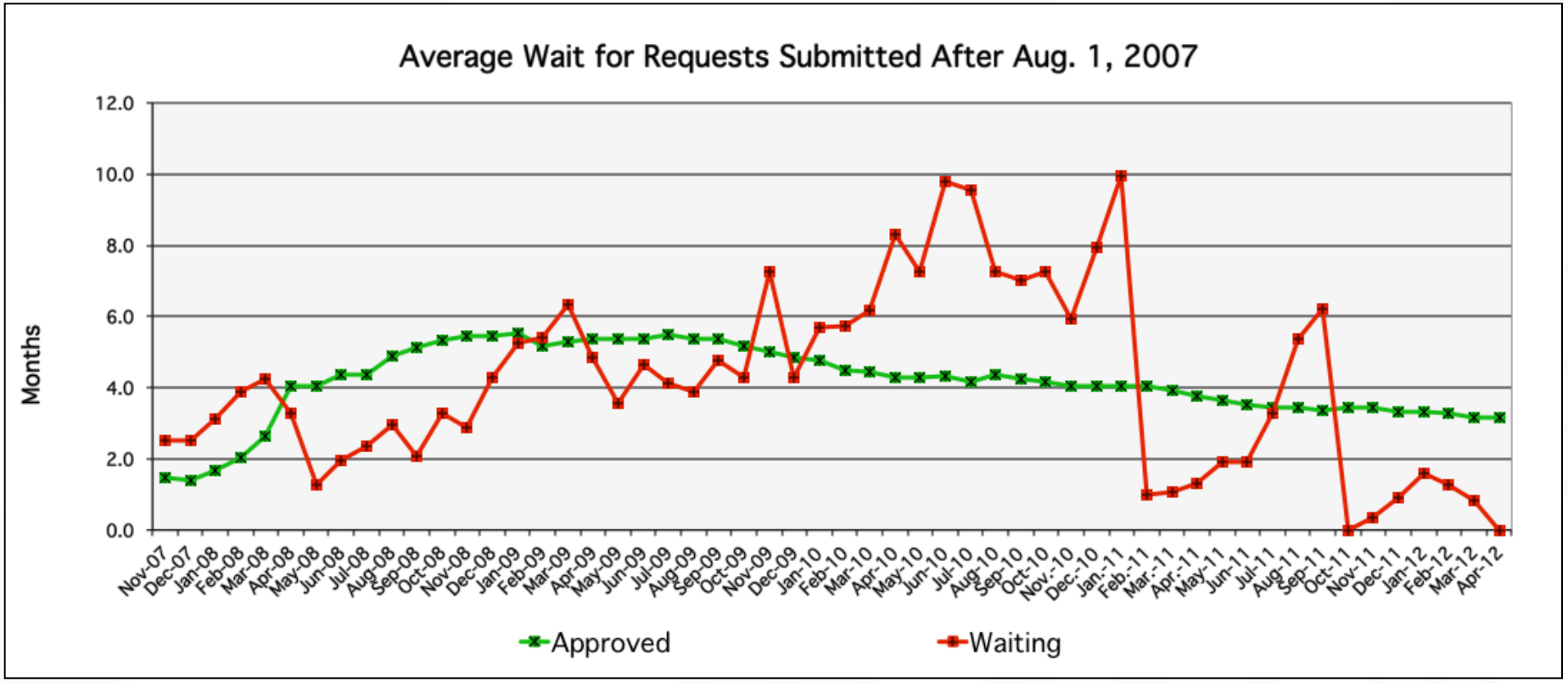
***Figure**: Noise-suppression technologies integrated into the rectangular nozzle architecture. Velocity contour predictions at takeoff by the Wind-US structured solver. Results shown are for a chevron nozzle with a 2:1 aspect ratio. Franco Frate, NASA/Glenn*

***POC:** Franco Frate, franco.c.frate@nasa.gov, (216) 433-8450, NASA Glenn Research Center*

** HECC provided supercomputing resources and services in support of this work.*

Status of Requests for NAS Computer Accounts by non-U.S. Citizens

- Requests approved: 3; New requests received: 2; Requests waiting: 0.
- The time to approval continues to improve. The three requests that were approved were approved in less than one month.



HECC Facility Hosts Several Visitors and Tours in March 2012

- HECC hosted 7 tour groups in March; guests learned about the Agency-wide missions being supported by Pleiades, and viewed scientific results on the hyperwall system. Visitors this month included:
  - 30 members from Marshall and Kennedy Space Flight Centers attending a Space Launch System Technical Interchange Meeting;
  - John Tracy, Chief Technology Officer for The Boeing Company;
  - 20 participants from the Naval Postgraduate School;
  - 15 University of Arizona students who are involved in the Exploration and Development of Space (SEDS) program;
  - 12 San Jose State University and AIAA students who are studying CFD related to vehicle reentry into the atmosphere.

Figure: *Students from the University of Arizona listen as Bryan Biegel, Deputy Chief of the NASA Advanced Supercomputing Division, describes a space exploration image shown on the hyperwall visualization system.*

POC: *Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division*

Presentations and Papers

- "High End Computing Capability Project: Enabling NASA Science and Engineering," William Thigpen, 3rd International Supercomputing Conference in Mexico, Mar. 14-16, Guanajuato, Mexico
  http://www.isum.mx
- "NASA Advanced Computing Environment for Science and Engineering," Rupak Biswas, 26th Annual HPCC Conference, Mar. 26-28, Newport, RI
  http://hpcc-usa.org/
- "Flow Analysis Tool Whitepaper," Nichole K. Boscia, NASA Advanced Supercomputing Facility report.
  http://www.nas.nasa.gov/publications/reports/reports.html
- "Parallel Jacobian-free Newton Krylov solution of the discrete ordinates method with flux limiters for 3D radiative transfer," William F. Godoy, Xu Liu, Journal of Computational Physics, Vol. 231, pp. 4257–4278, available online February 24, 2012.*
  http://dx.doi.org/10.1016/j.jcp.2012.02.010
- "Planetesimal and Protoplanet Dynamics in a Turbulent Protoplanetary Disk: Ideal Stratified Disks," CC Yang, MM Mac Low, The Astrophysical Journal, Vol. 748, Number 2, February 9, 2012.*
  http://iopscience.iop.org/0004-637X/748/2/79/
- "Continental scale, high order, high spatial resolution, ice sheet modeling using the Ice Sheet System Model (ISSM)," E. Larour, H. Seroussi, M. Morlighem, E. Rignot, Journal of Geophysical Research, Vol. 117, F01022, 2012.*
  http://www.agu.org/pubs/crossref/2012/2011JF002140.shtml
- "Sensitivity analysis of Pine Island Glacier ice flow using ISSM and DAKOTA," E. Larour, J. Schiermeier, E. Rignot, H. Seroussi, et al, Journal of Geophysical Research, Vol. 117, F01022, 2012.*
  http://www.agu.org/pubs/crossref/pip/2011JF002146.shtml

** HECC provided supercomputing resources and services in support of this work.*

News and Events

- **Steve Legensky to Discuss Small Manufacturer Success at HPCC,** *HPCwire*, March 23, 2012 – Feature article mentioning Rupak Biswas' participation in the National High Performance Computer and Communications Council March 26-28 in Newport, Rhode Island.
  http://www.hpcwire.com/hpcwire/2012-03-22/steve_legensky_to_discuss_small_manufacturer_success_at_hpcc.html

- **Kepler Mission Manager Update**, *Kepler Mission News,* March 22, 2012 – Includes information on visualization expert Chris Henze's participation in a Kepler presentation on the hyperwall; picked up by various media sources, including *Space Fellowship*.
  http://www.nasa.gov/mission_pages/kepler/news/keplerm-20120322.html

- **Engineers Enlist Weather Model to Optimize Offshore Wind Plan**, *Stanford University School of Engineering News,* March 21, 2012 – Using a sophisticated weather model, environmental engineers at Stanford University have defined optimal placement of a grid of four wind farms off the U.S. East Coast. HECC provided access to computational resources at the NASA Advanced Supercomputing facility.
  http://environmentalresearchweb.org/cws/article/yournews/49108

- **Supercomputing Conference Held in Guanajuato**, *El Universal Mx,* March 13, 2012 – Announcement highlighting participation of Bill Thigpen in international HEC conference; similar announcements covered in *Alianza* and other Spanish language publications.
  http://www.eluniversal.com.mx/articulos/69632.html

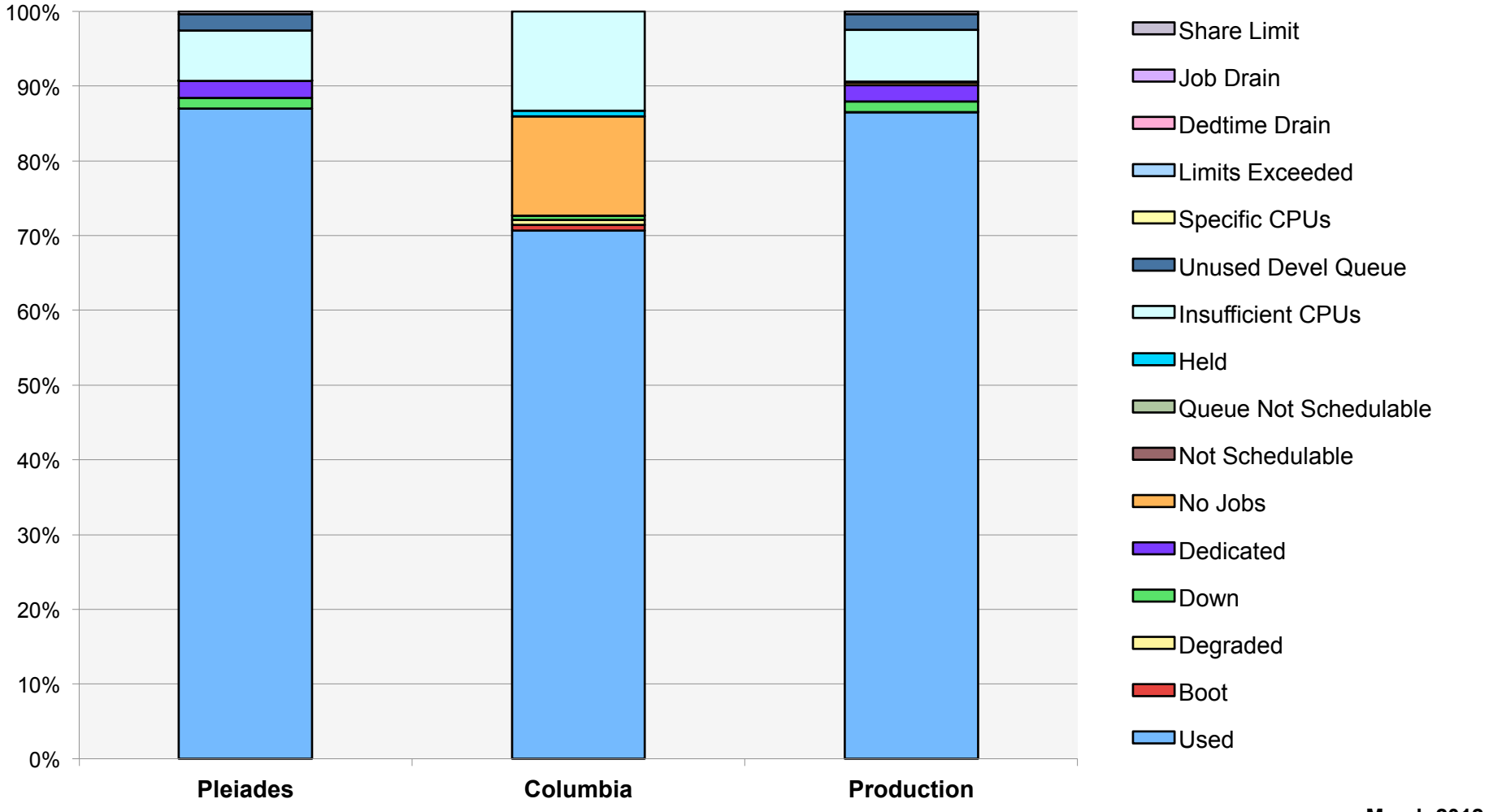
News and Events (cont.)

- **Media Invited to Apply for UC-HiPACC Journalism Boot Camp on Computational Astronomy,** *SpaceRef*, March 12, 2012 – News item on journalist field trip to NASA Ames to see the Pleiades supercomputer and the 128-screen hyperwall. http://www.spaceref.com/news/viewpr.html?pid=36371

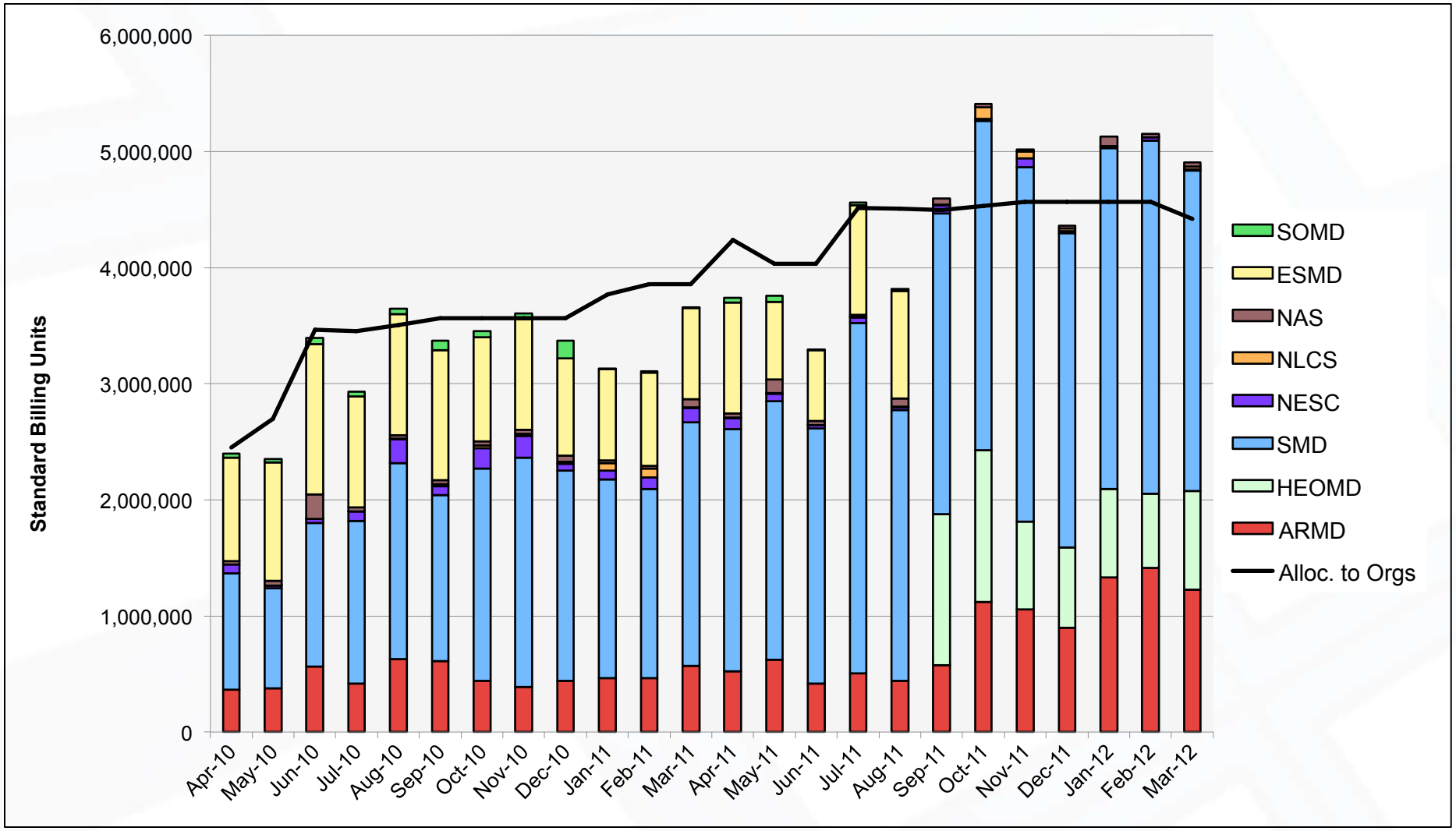
- **Rogue Wave Software Sets a New Standard for Debugging**, Rogue Wave Software *press release*, March 6, 2012 – Quotes HECC scientific consult Johnny Chang on use of TotalView Software. Picked up numerous media sources, including MSNBC, MarketWatch, http://www.roguewave.com/company/news-events/press-releases/2012/a-new-standard-for-debugging.aspx

- **Petaflop Computing for the Masses – SGI and the Intel Xeon Processor E5 Family – Intel Chip Chat – Episode 175,** *Connected Social Media: The Intel Channel,* In this Intel Chip Chat audio podcast with Allyson Klein: Bill Mannel from SGI and Bill Thigpen from NASA discuss the launch of SGI ICE X based on the Intel Xeon processor E5 family and using high end computing at NASA for things like exploring space or looking at how we're affecting our environment. http://connectedsocialmedia.com/intel/5720/petaflop-computing-for-the-masses-sgi-and-the-intel-xeon-processor-e5-family-intel-chip-chat-episode-175/

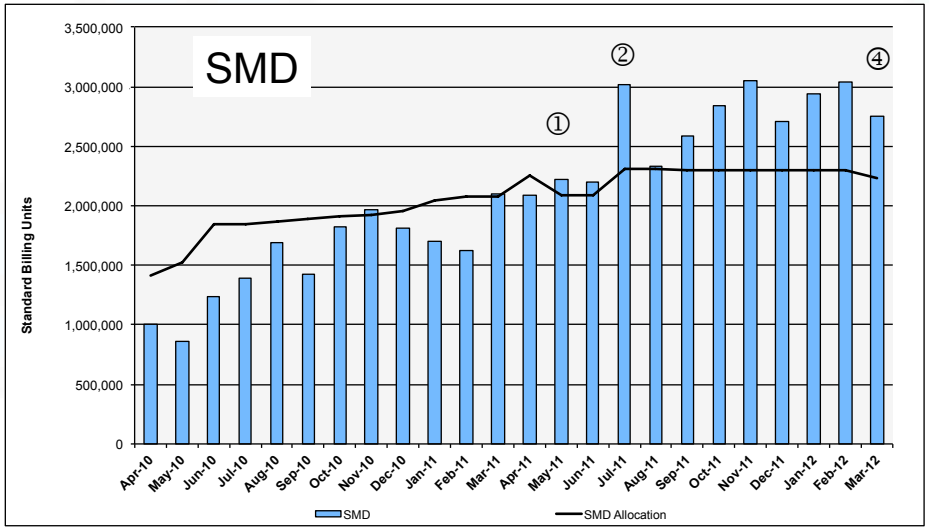
HECC Utilization

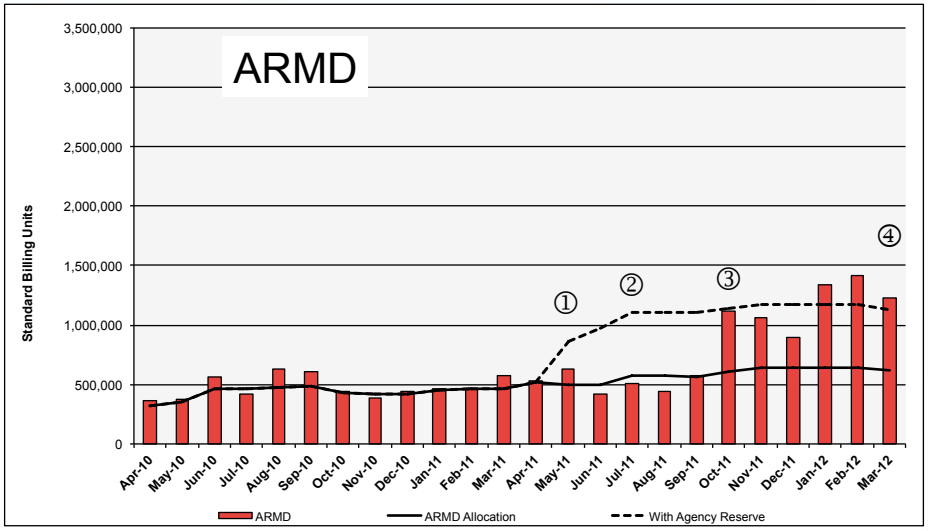


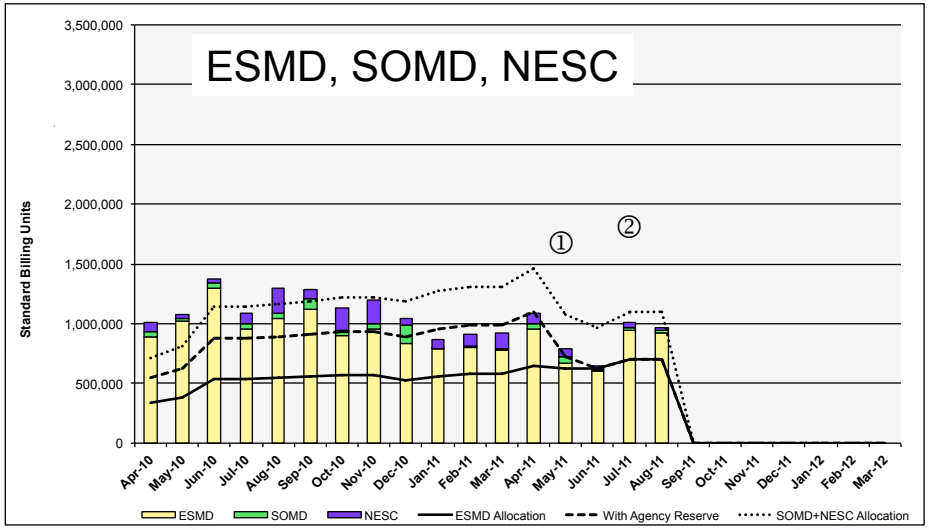
HECC Utilization Normalized to 30-Day Month

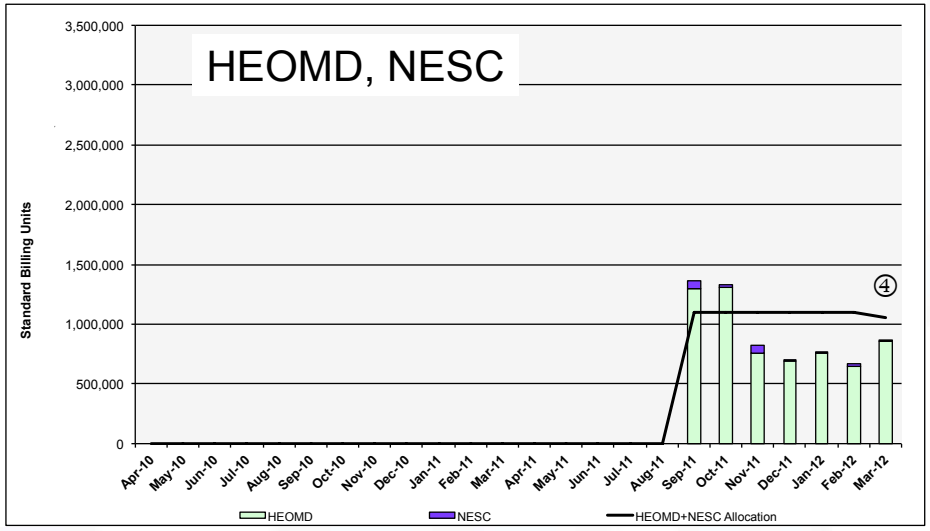


HECC Utilization Normalized to 30-Day Month



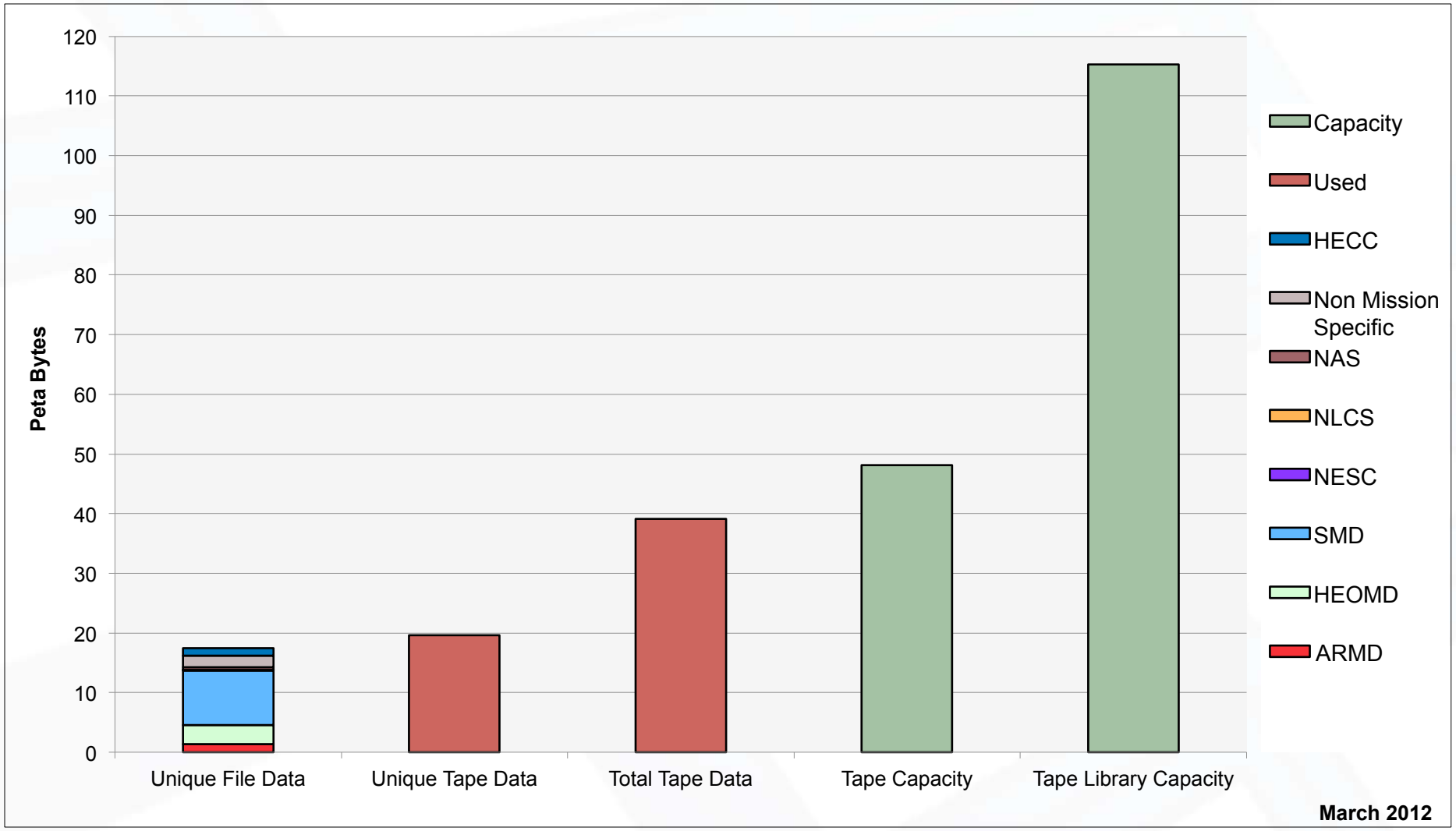






① Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD ② 14 Westmere racks added
③ 2 ARMD Westmere racks added ④ 28 Harpertown racks removed

Tape Archive Status



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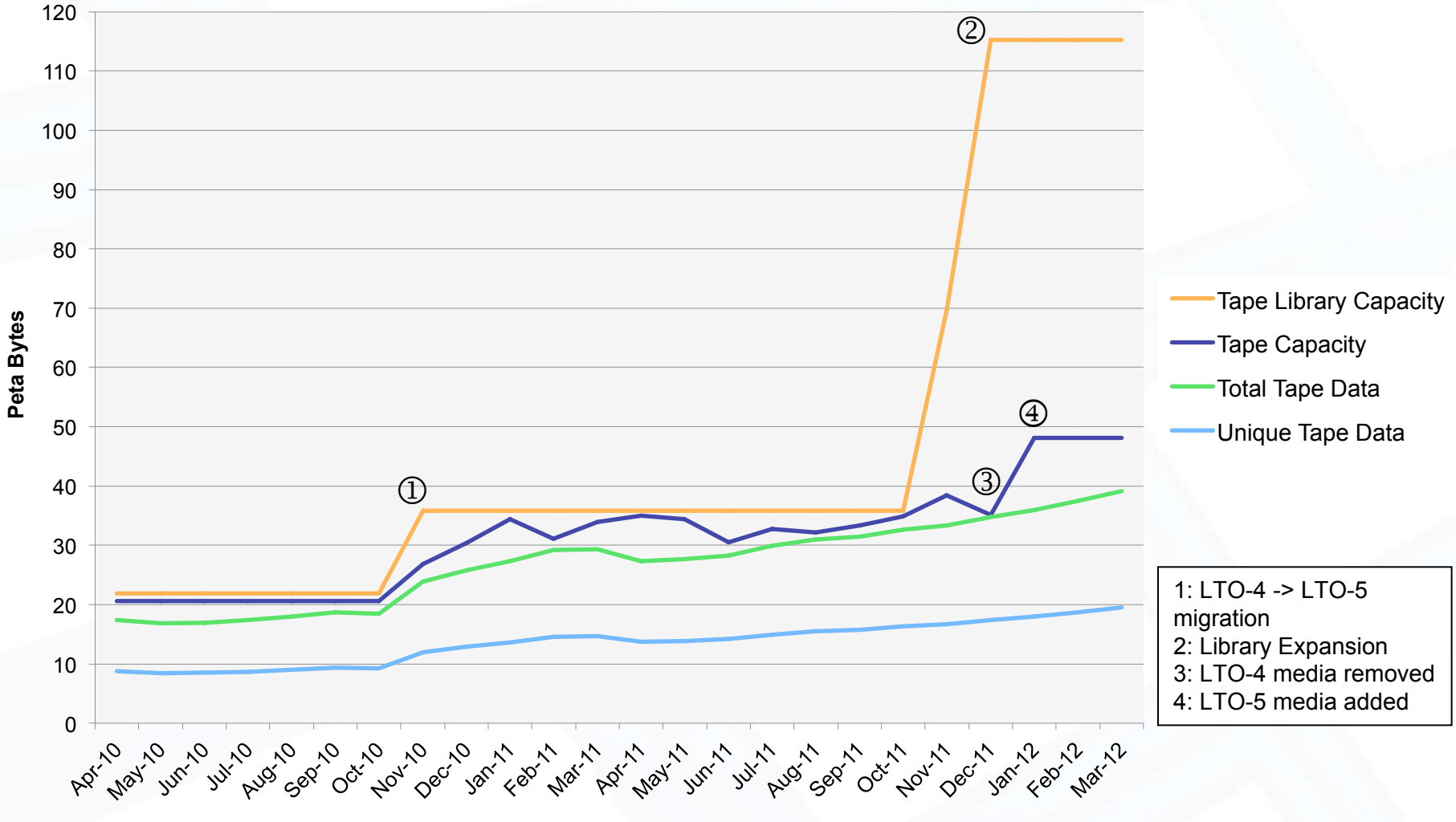
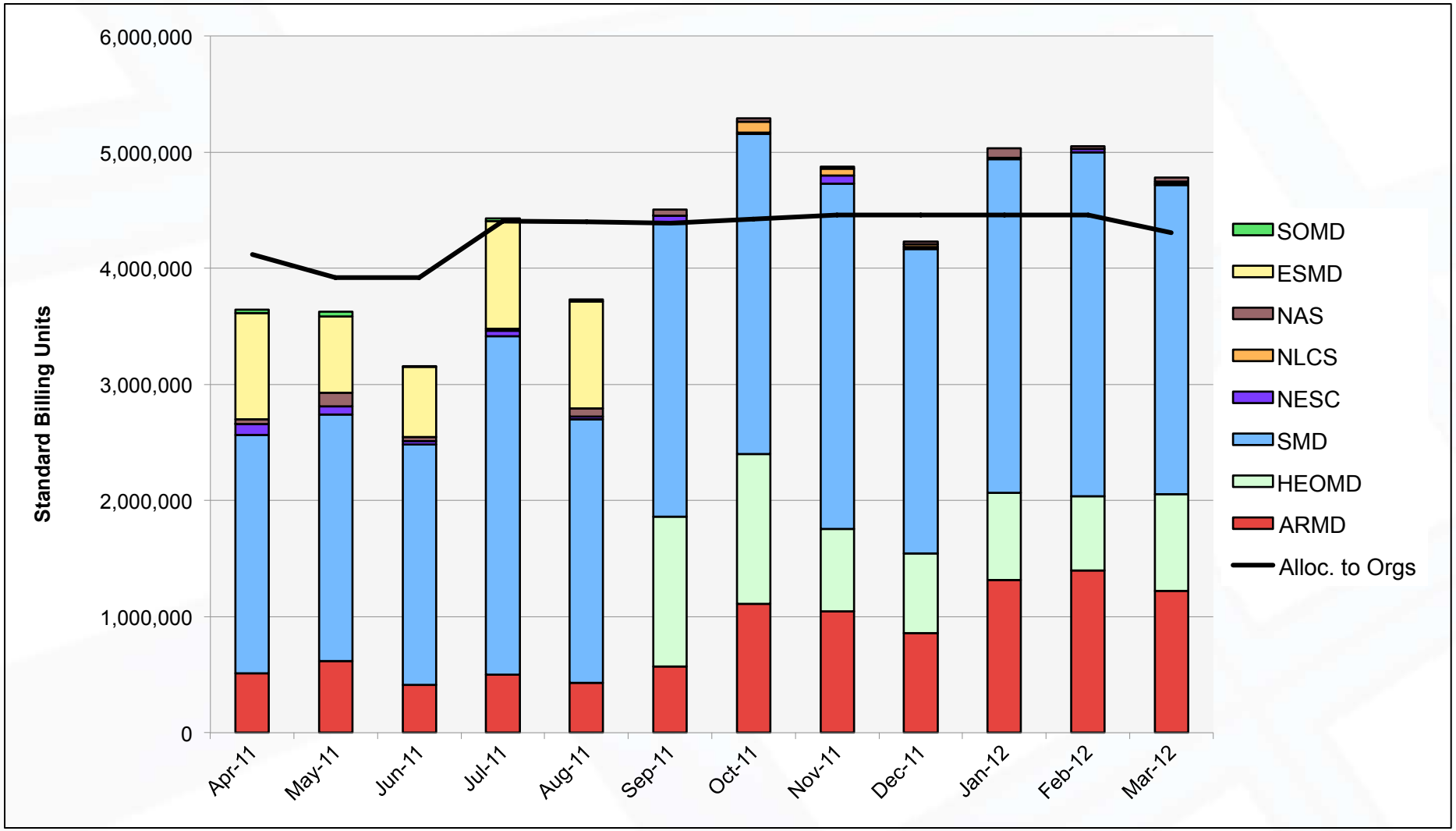
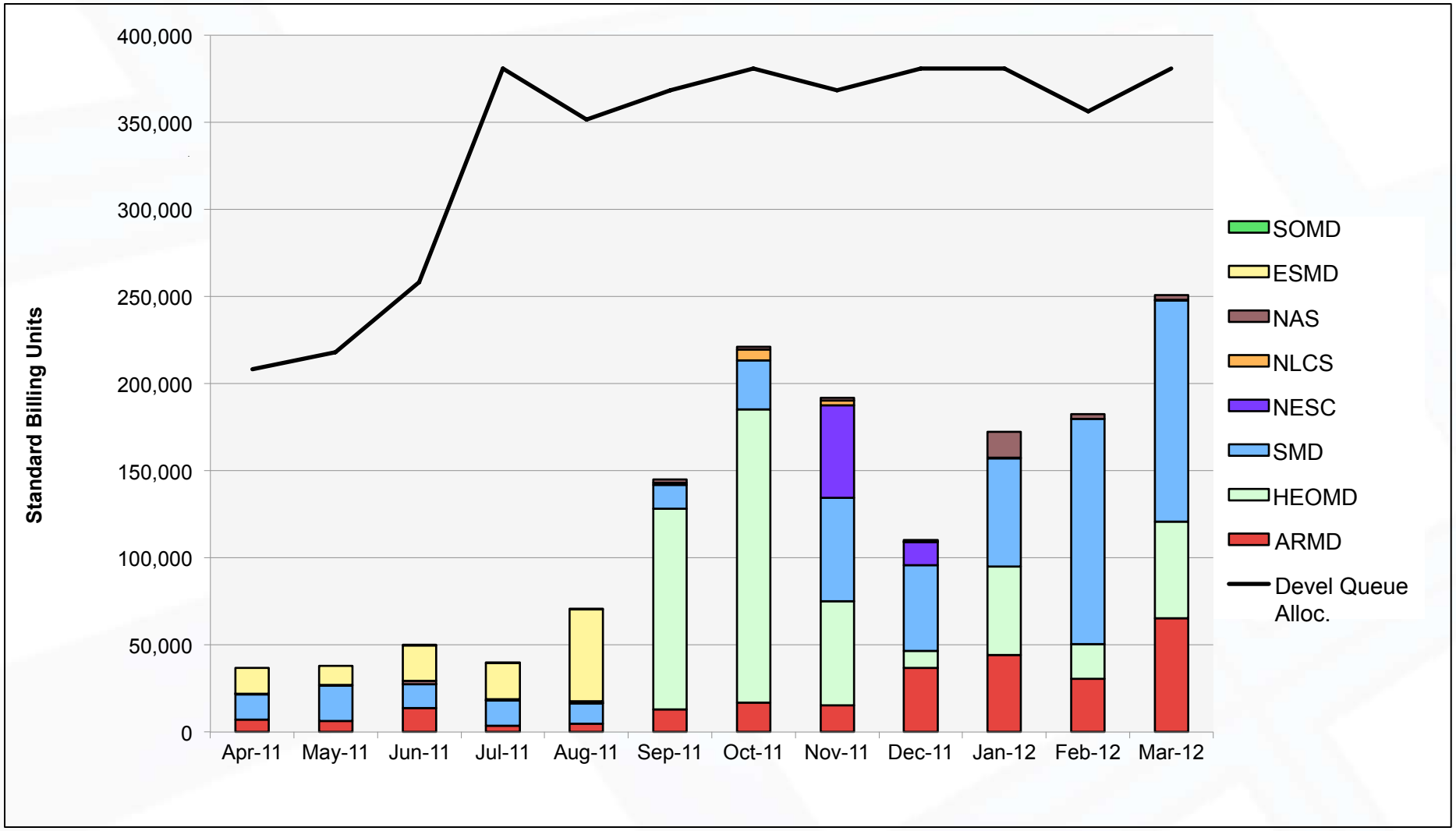


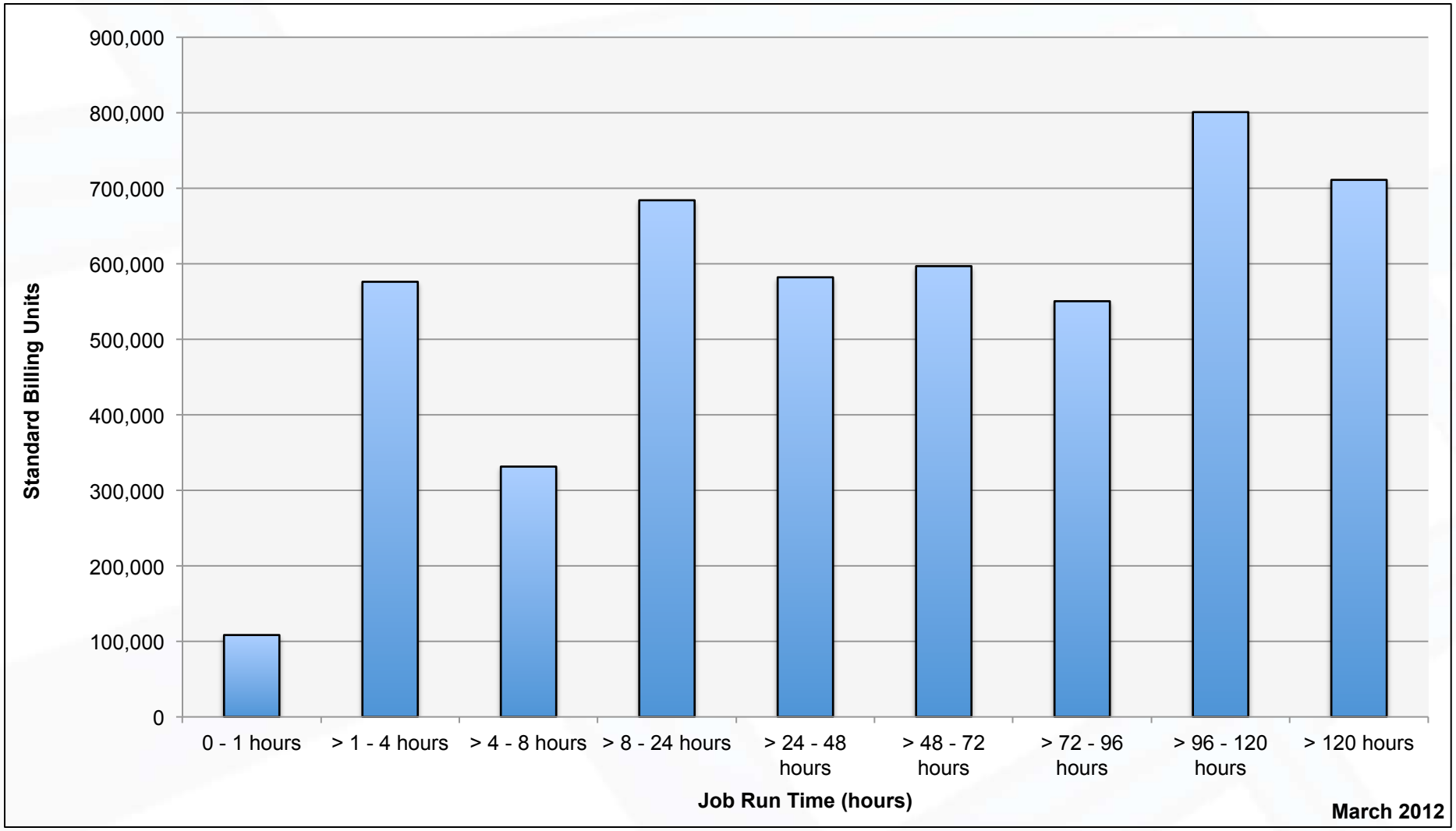
Pleiades:
SBUs Reported, Normalized to 30-Day Month



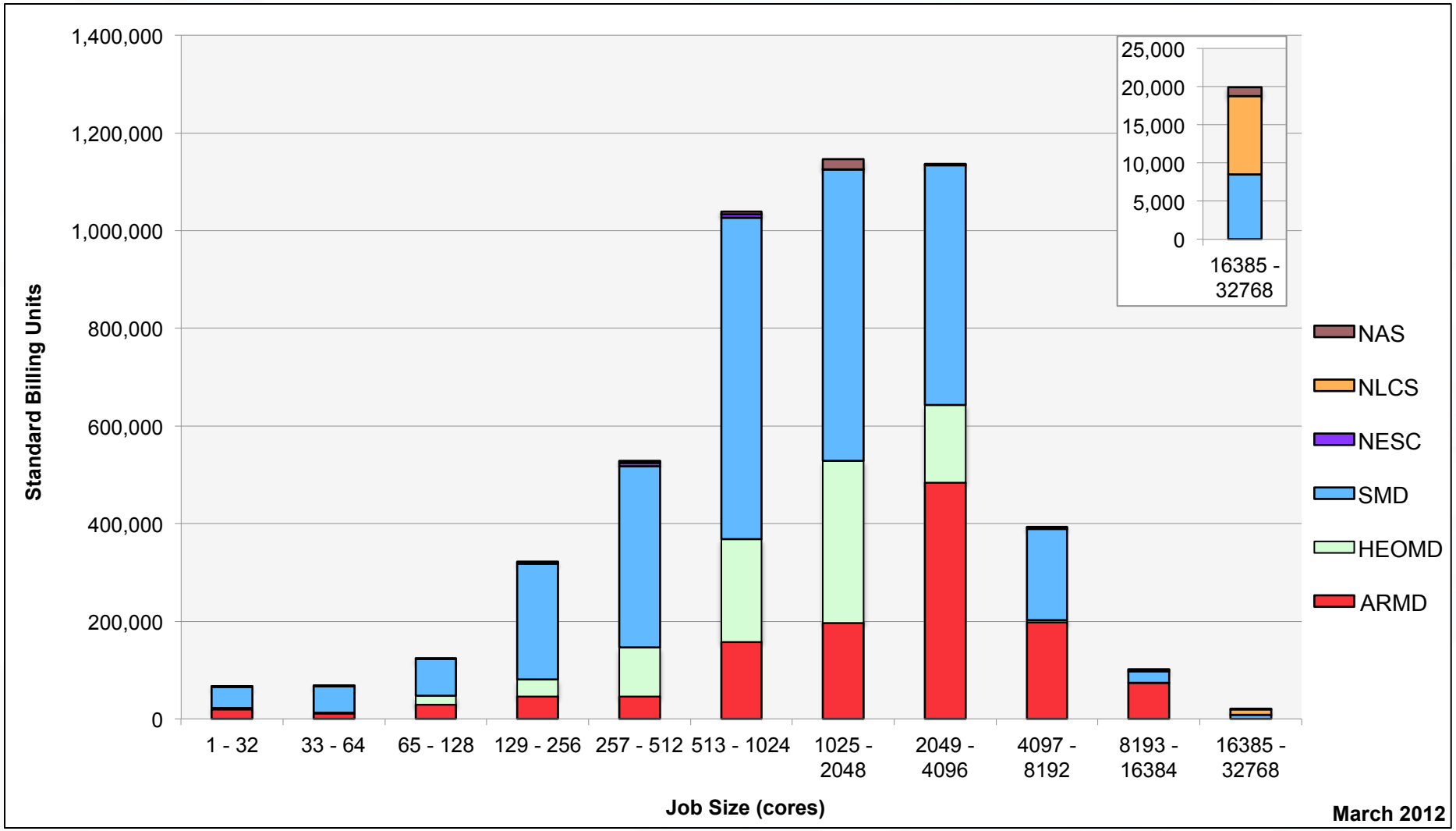
Pleiades:
Devel Queue Utilization



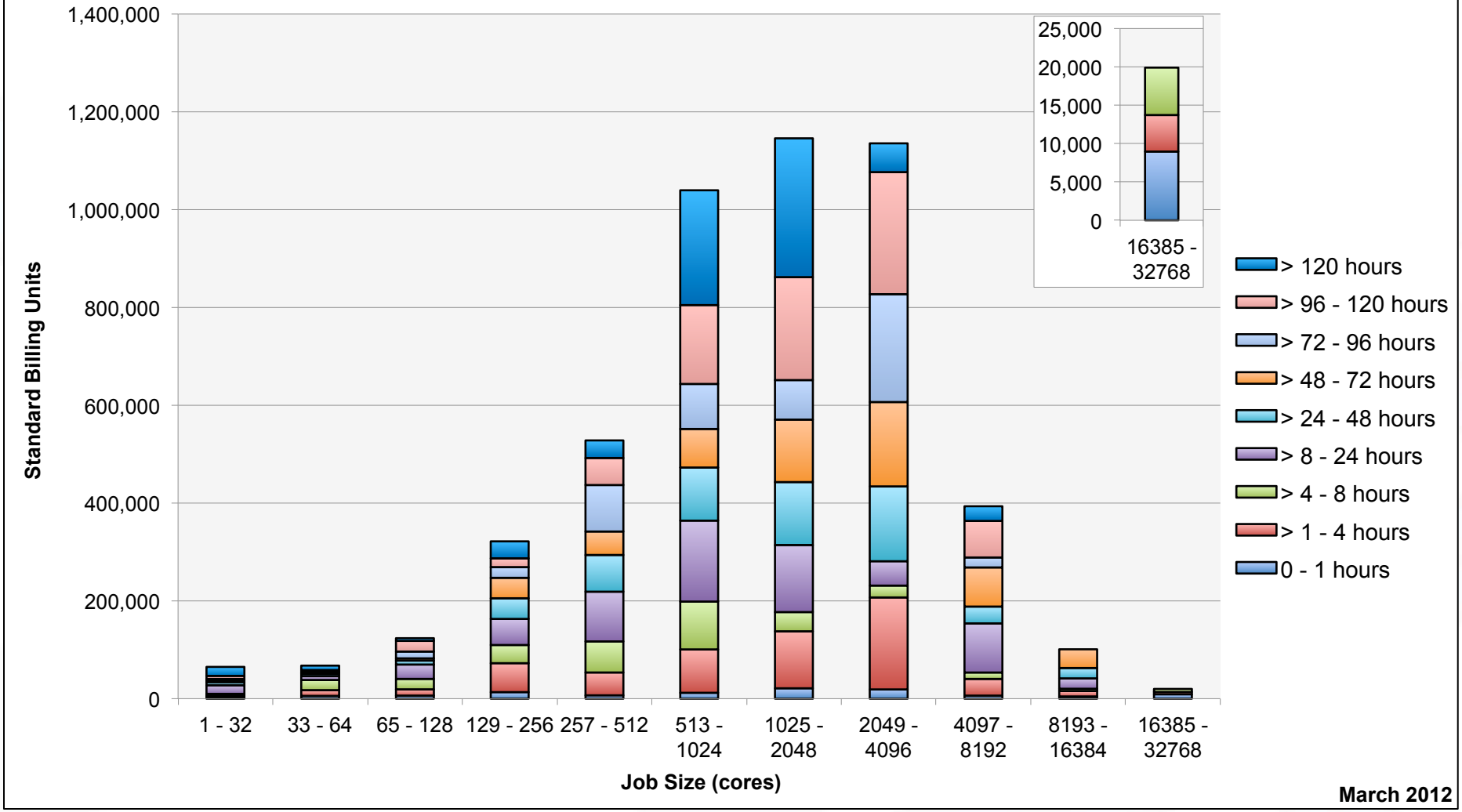
Pleiades:
Monthly SBUs by Run Time



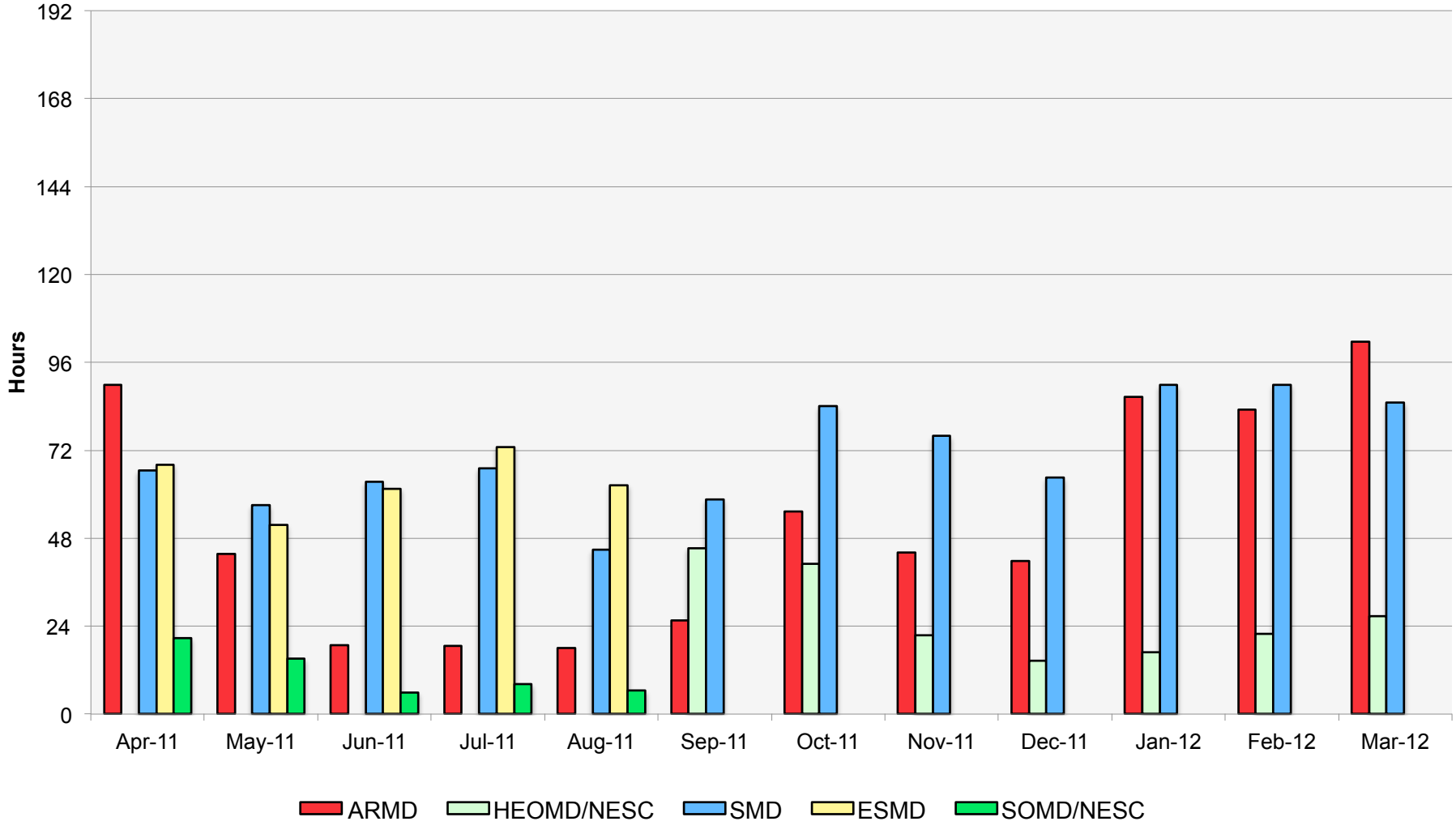
Pleiades:
Monthly Utilization by Size and Mission



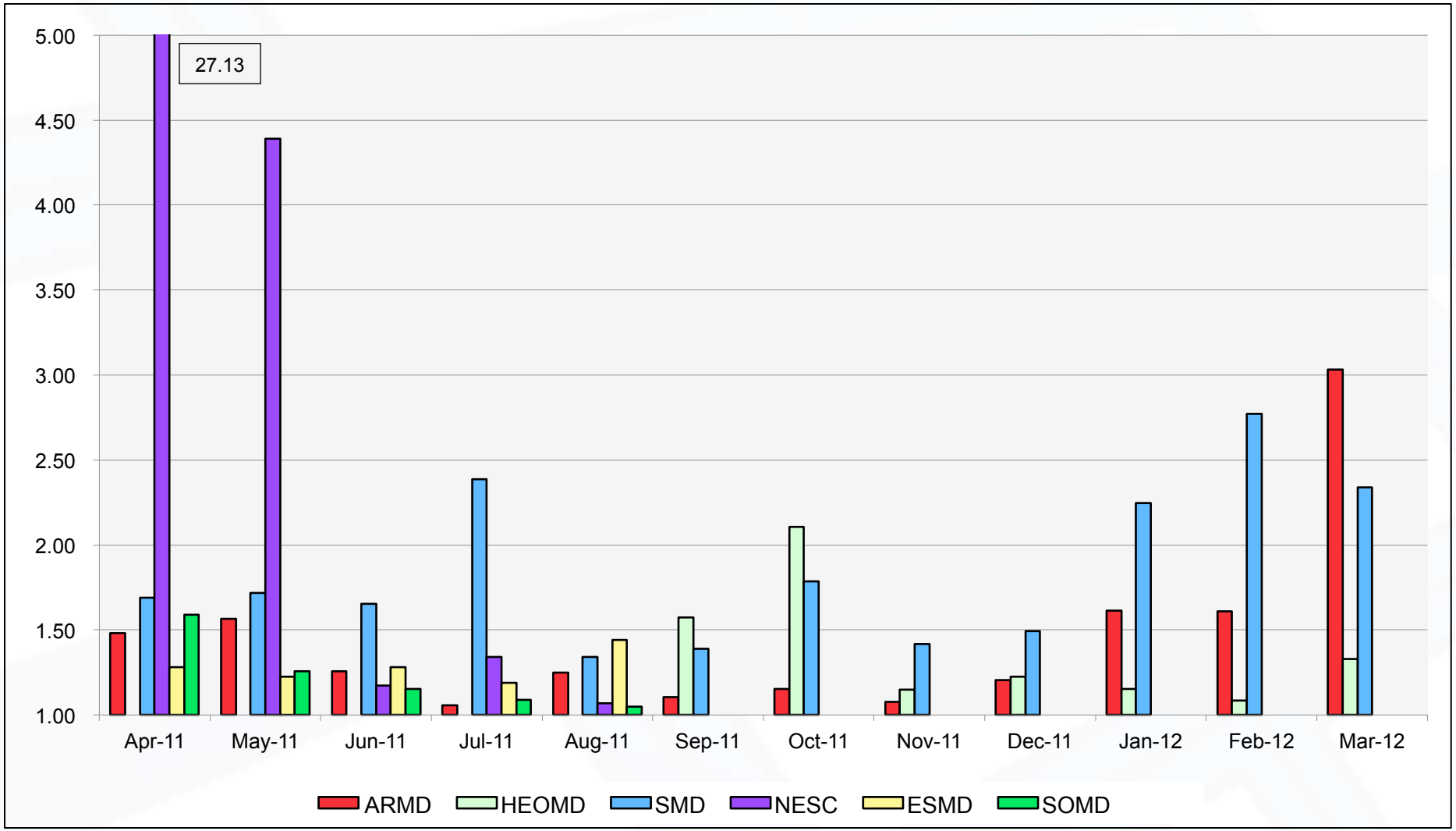
Pleiades:
Monthly Utilization by Size and Length



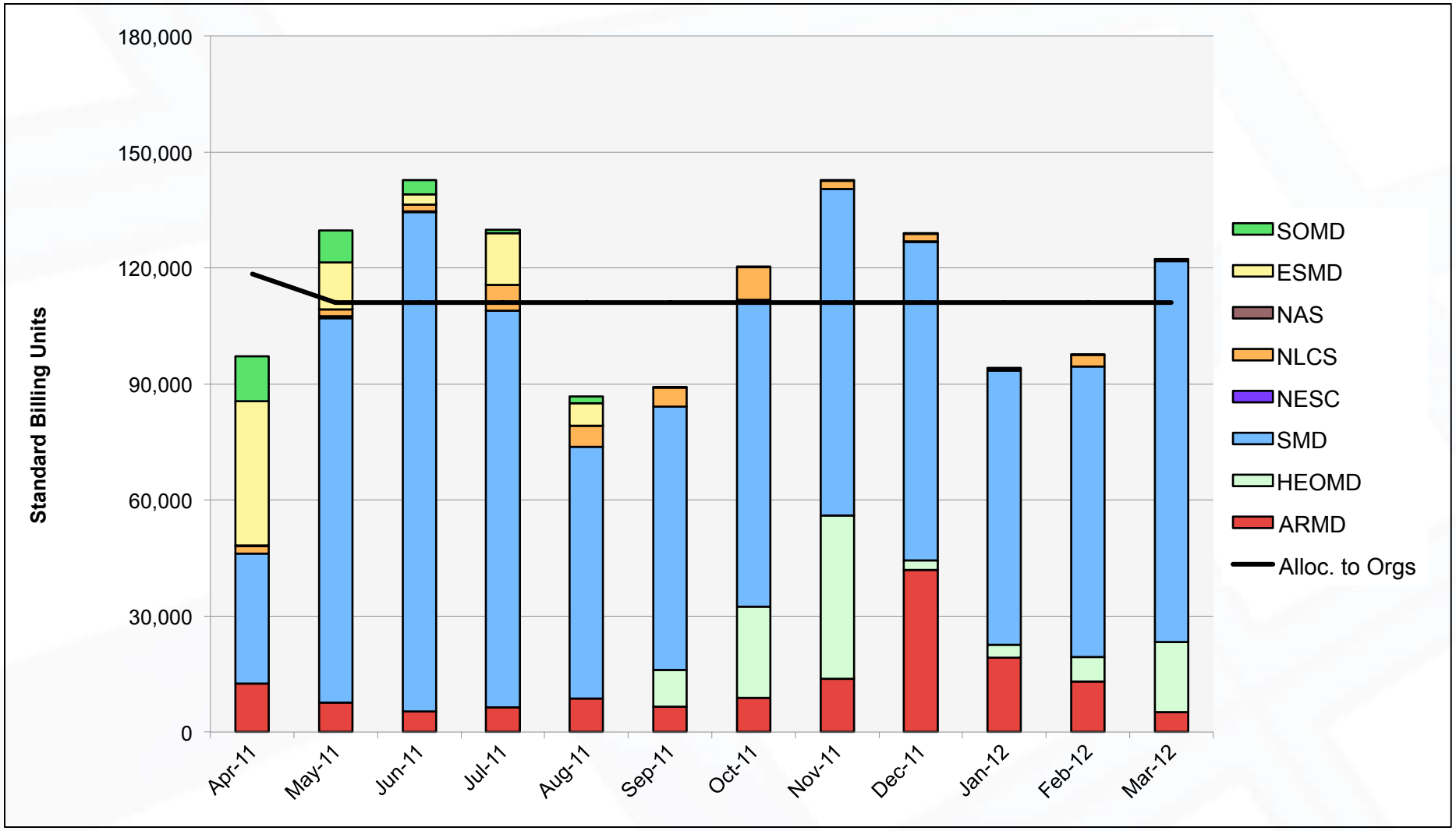
Pleiades:
Average Time to Clear All Jobs



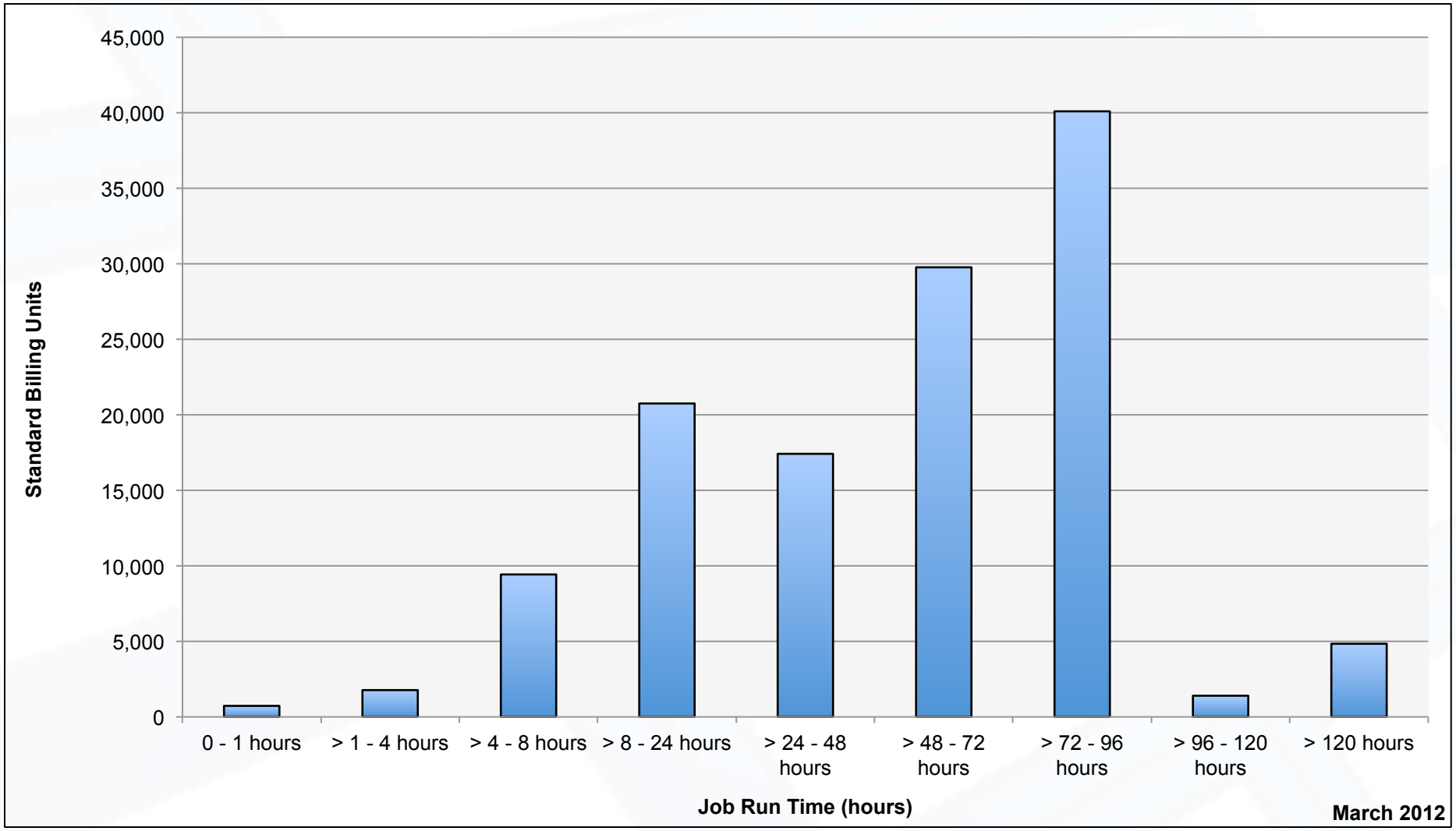
Pleiades:
Average Expansion Factor



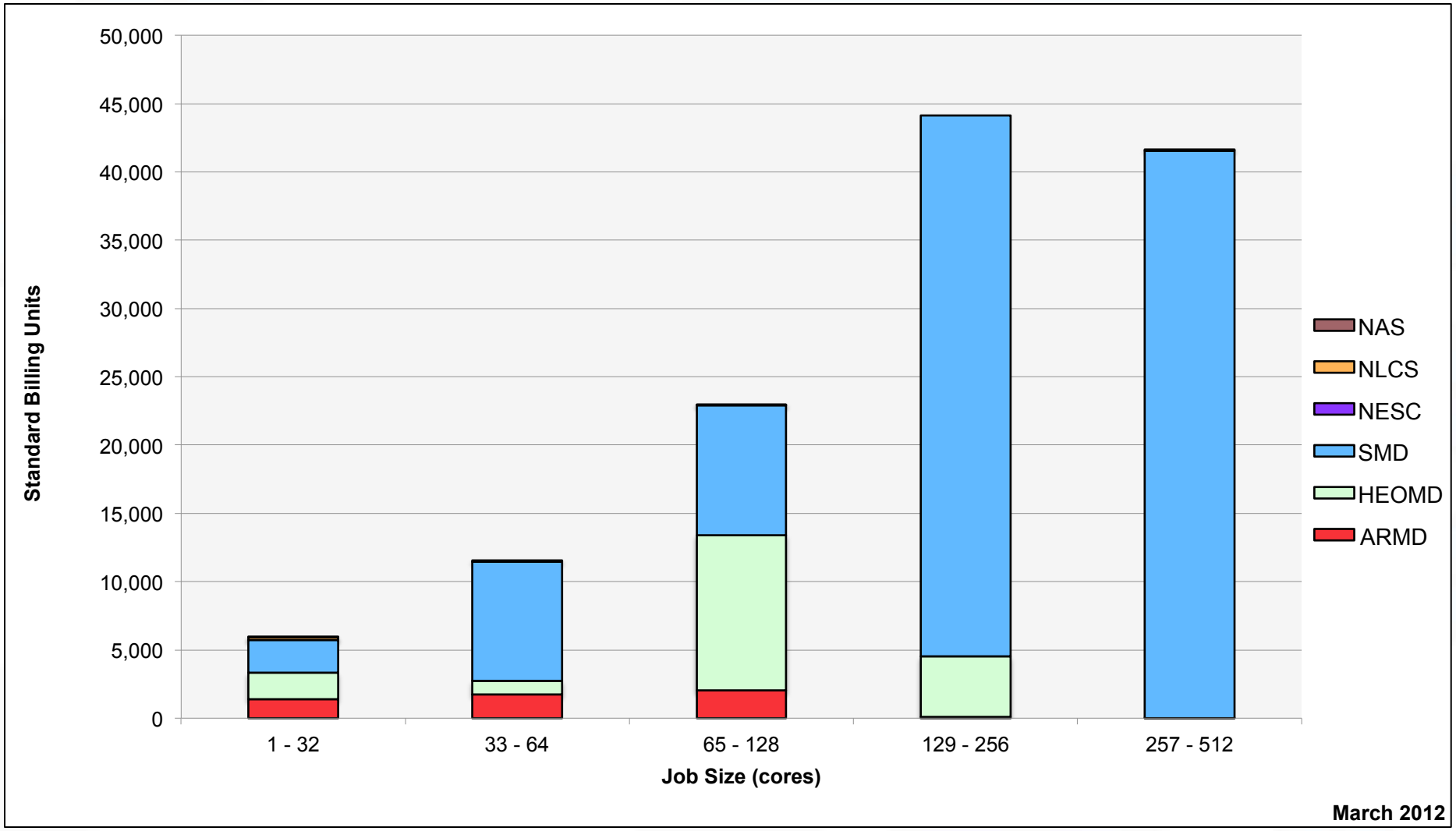
Columbia:
SBUs Reported, Normalized to 30-Day Month



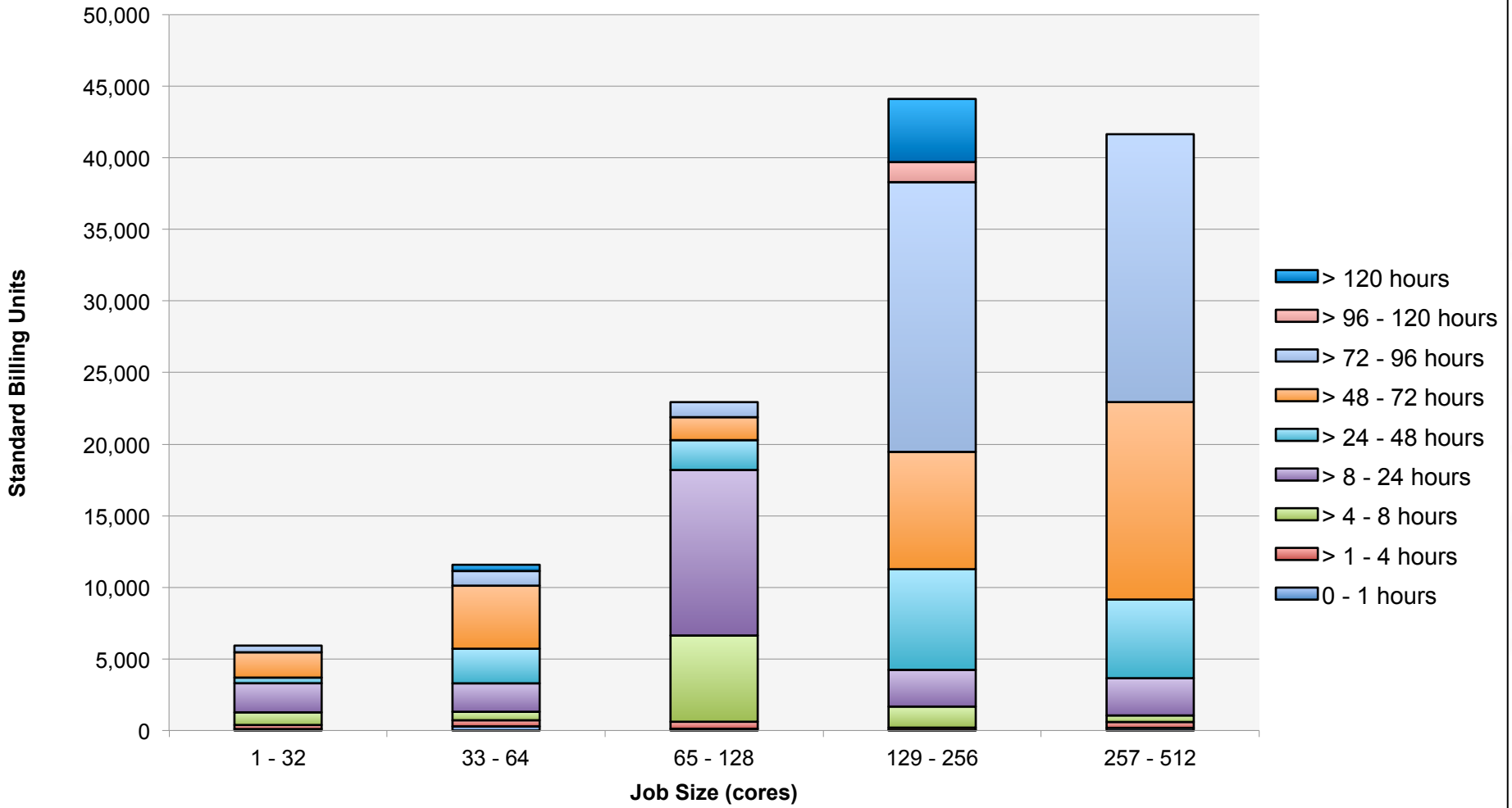
Columbia:
Monthly SBUs by Run Time



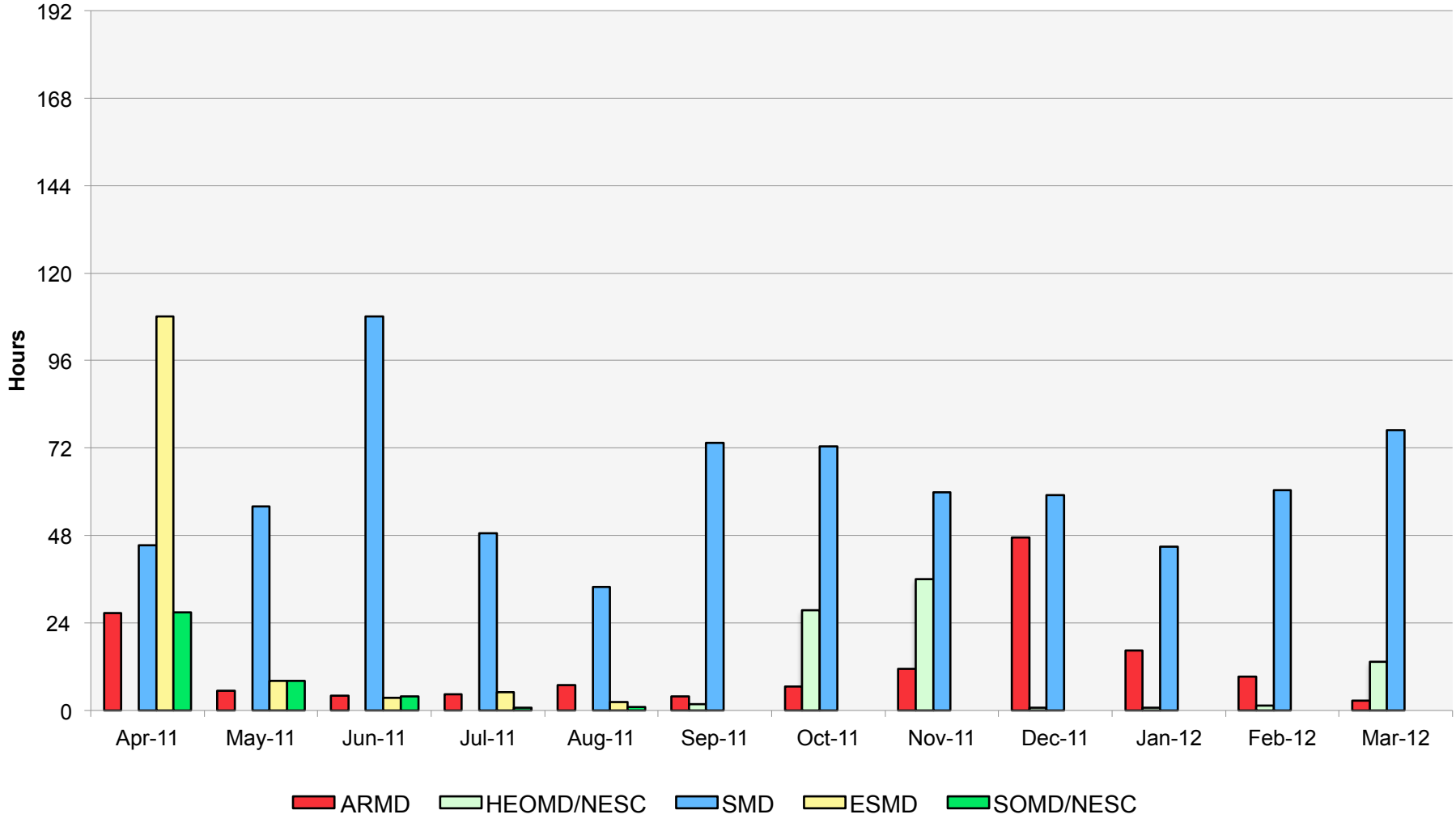
Columbia:
Monthly Utilization by Size and Mission



Columbia:
Monthly Utilization by Size and Length



Columbia:
Average Time to Clear All Jobs



Columbia:
Average Expansion Factor